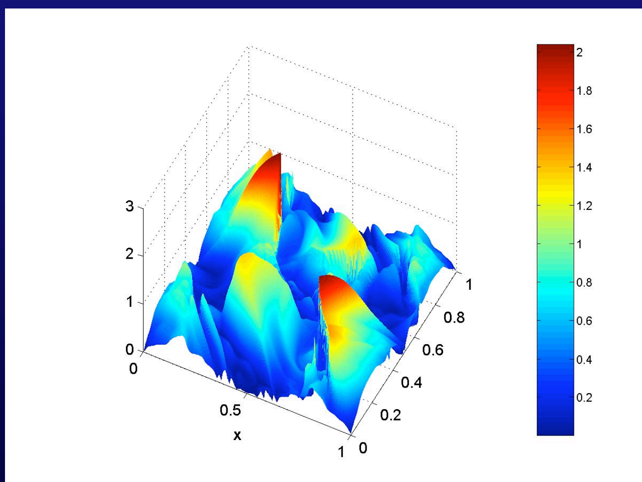
Algorithms and Comparisons of Compressible Magnetohydrodynamic Flows



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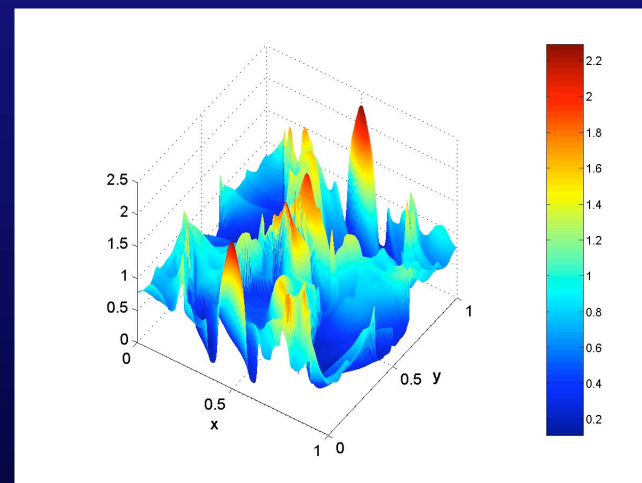

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Goddard Space Flight Center
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Outline of Presentation

- **Introduction:**
  - Descriptions of 1D & 2D MHD problems.
  - Motivation of the scheme.
  - Difficulties in efficient numerical solution to ensure solenoidal magnetic fields.
- **Mathematical and numerical Implementations:**
  - Governing equations in a conservative form.
  - Staggered mesh algorithm.
  - Riemann problem.
    - Roe-Type scheme, FOG & HOG, TVD.
    - Dimensional splittings.
- **Code structure and computation.**
- **Results & discussion.**
  - Methodology, validation and analysis of results.
- **References.**

1D & 2D MHD problems

1D problem

- Brio-Wu's 1.5D ideal MHD problem.
- All variables are functions of x only.
- Vector quantities with perpendicular direction.
- B_x is constant.
- $\nabla \cdot \vec{\mathbf{B}} = 0$ is trivial.
- Nonlinear, 5-component PDE, 5 conserved variables.
- 5 wave Riemann problem.
- e.g., Fast rarefaction wave, slow compound wave (shock+rarefaction), contact discontinuity, slow shock, fast rarefaction wave.

2D problem

- Orszag-Tang's MHD vortex problem.
- One more variable in y direction.
- Vector quantities with normal and tangential directions for each sweeps.
- B_x is not a constant.
- $\nabla \cdot \vec{\mathbf{B}} = 0$ is a new restriction!
- 7 wave Riemann problem.
- e.g., Fast rarefaction wave, Alfven wave, slow rarefaction wave, contact discontinuity, slow shock, Alfven wave, fast shock wave.
- More complicated wave structures with a numerical restriction.

Numerical MHD

- Three approaches for ensuring $\nabla \cdot \vec{\mathbf{B}} = 0$ with high order Godunov types solver:
  - 8-wave, projection scheme, & CT / CD.
- 8-wave (Powell et al., 1999)
  - can spoil conservation (incorrect jump conditions across discont.)
  - keeps $\nabla \cdot \vec{\mathbf{B}} = 0$ to the accuracy of truncation error, i.e., requires zero divergence to be satisfied to the 2^{nd} order accuracy in IC & BC.
- Projection scheme (Brackbill and Barnes, 1980, Crockett et al., 2003)
  - keeps $\nabla \cdot \vec{\mathbf{B}} = 0$ to the accuracy of the Poisson solver.
  - accurate but expensive.
- CT scheme using staggered algorithm (Evans and Hawley, 1988, Balsara and Spicer, 1999)
  - maintains $\nabla \cdot \vec{\mathbf{B}} = 0$ to the accuracy of machine round off errors.
  - same order of accuracy as the projection scheme.
- Extensive tests and comparisons are made by Toth [3].

Conservation Form of Ideal MHD Equations (2D)

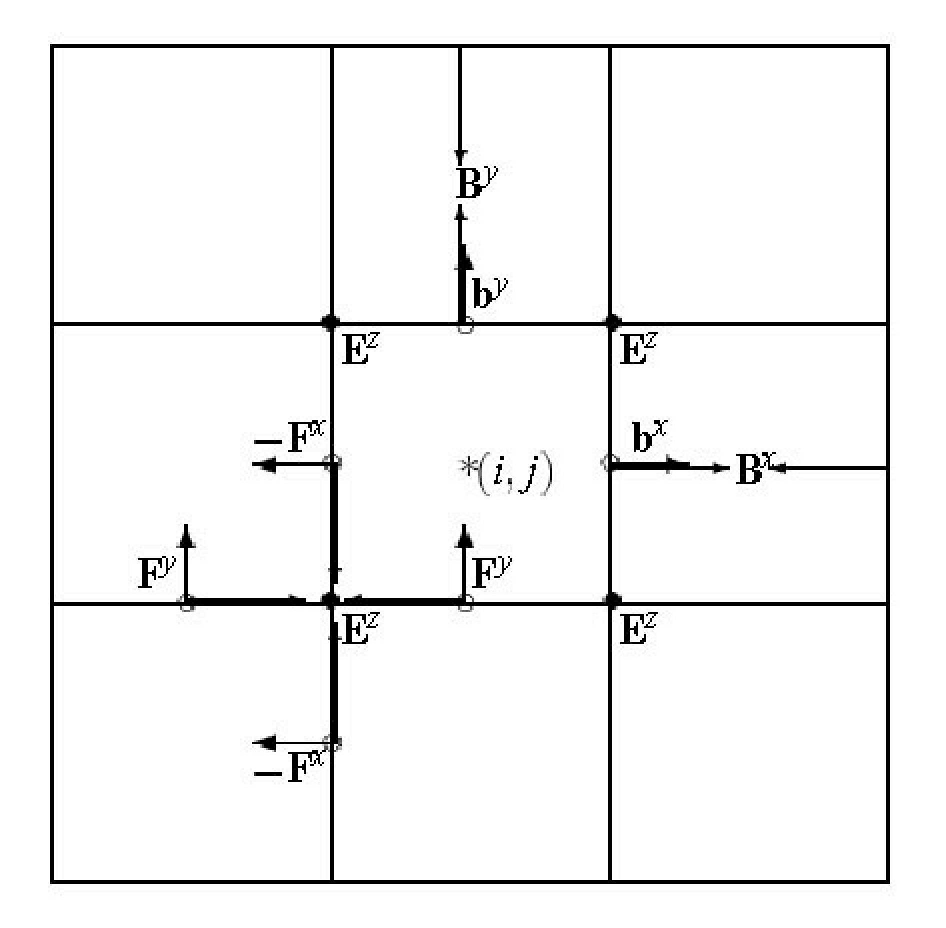
- The ideal MHD governing equations in 2D : $\dfrac{\partial \vec{\mathbf{U}}}{\partial t} + \dfrac{\partial \vec{\mathbf{F}}}{\partial x} + \dfrac{\partial \vec{\mathbf{G}}}{\partial y} = 0$

$$\vec{\mathbf{U}} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ B_x \\ B_y \\ B_z \\ E \end{pmatrix} \qquad \vec{\mathbf{F}} = \begin{pmatrix} \rho u \\ \rho u^2 + P^* - B_x{}^2 \\ \rho uv - B_x B_y \\ \rho uw - B_x B_z \\ 0 \\ uB_y - vB_x \\ uB_z - wB_x \\ (E + P^*)u - B_x(uB_x + vB_y + wB_z) \end{pmatrix} \qquad \vec{\mathbf{G}} = \begin{pmatrix} \rho v \\ \rho uv - B_x B_y \\ \rho v^2 + P^* - B_y{}^2 \\ \rho vw - B_y B_z \\ vB_x - uB_y \\ 0 \\ vB_z - wB_y \\ (E + P^*)v - B_y(uB_x + vB_y + wB_z) \end{pmatrix}$$

$$E = \frac{p}{\tilde{a}-1} + \frac{\tilde{n}}{2}\left(u^2 + v^2 + w^2\right) + \frac{1}{2}\left(B_x^2 + B_y^2 + B_z^2\right) \qquad P^* = p + \frac{1}{2}\left(B_x^2 + B_y^2 + B_z^2\right)$$

Staggered Mesh Algorithm

- 2D staggered grid topology to ensure $\nabla \cdot \vec{\mathbf{B}} = 0$.
- Upwinded fluxes $\vec{\mathbf{F}}$ collocated at centers of cell interfaces.
- $\dot{\vec{\mathbf{A}}} = -\vec{\mathbf{v}} \times \vec{\mathbf{A}}$ at cell corners.
- Algorithm:
  - IC & BC for $\nabla \cdot \vec{\mathbf{b}} = 0$
  - $\vec{\mathbf{F}}$ from high order Godunov
  - Update $\vec{\mathbf{E}}$ using $\vec{\mathbf{F}}$
  - Update $\vec{\mathbf{b}}$ using Maxwell's 3rd eqn:
    $$\partial_t \vec{\mathbf{b}} + \nabla \cdot \vec{\mathbf{E}} = 0$$
  - Update $\vec{\mathbf{B}}$ by interpolating $\vec{\mathbf{b}}$



Staggered Mesh Algorithm – cont'd

- Using the staggered mesh algorithm, one can maintain the discretized numerical divergence of magnetic fields remain zero!

$$(\nabla \cdot \mathbf{b})_{(i,j)}^{n+1} = \frac{b_{(i+1/2,j)}^{x,n+1} - b_{(i-1/2,j)}^{x,n+1}}{\Delta x} + \frac{b_{(i,j+1/2)}^{y,n+1} - b_{(i,j-1/2)}^{y,n+1}}{\Delta y} = 0\,,$$

$$\text{provided } (\nabla \cdot \mathbf{b})_{(i,j)}^{n} = 0$$

- Important constraint in MHD problems whose dimensionality > 1.
- $\nabla \cdot \vec{\mathbf{B}} \neq 0$ can be generated even with solenoidal IC & BC, due to inherent non-linearities of many shock-capturing numerical methods.
- If not controlled then the build-up of non-zero magnetic fields will yield numerical instability without any physical meanings.

Riemann Solver for Nonlinear MHD

- **Required for Godunov type methods.**

- **Approximate Riemann solvers are faster and efficient.**
  - Roe-type upwind differencing scheme.
  - Roe's linearization procedure.
  - Construction of a Roe matrix, $\overline{\mathbf{A}}$.
    - Analytical form is available at $\gamma = 2$ (Brio & Wu [5]).
    - Simple arithmetic averaging for $\gamma \neq 2$.
  - Use eigensystem of a Roe matrix to compute numerical fluxes at cell interface centers.

Roe's Linearization

$$\vec{\mathbf{U}}_t + \vec{\mathbf{F}}(\vec{\mathbf{U}})_x = 0 \quad \Rightarrow \quad \begin{aligned} &\vec{\mathbf{U}}_t + \overline{\mathbf{A}}\mathbf{U}_x = 0, \\ &\overline{\mathbf{A}} = \overline{\mathbf{A}}(\mathbf{U}_\mathbf{L}, \mathbf{U}_\mathbf{R}) = \overline{\mathbf{A}}(\mathbf{V}_0) \end{aligned}$$

Properties of $\overline{\mathbf{A}}$ ***:***

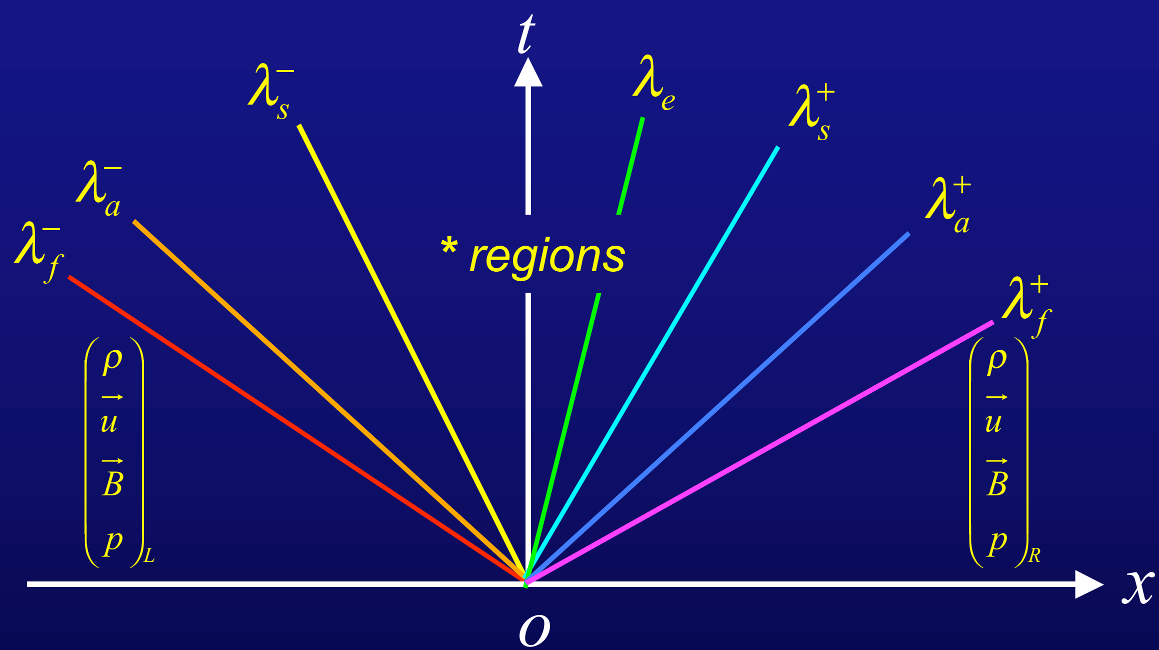
- **Hyperbolicity: (may not be strictly hyperbolic)**
  - $\overline{\mathbf{A}}$ is required to have real eigenvalues and linearly independent right eigenvectors.
- **Consistency with exact Jacobian:**

$$\overline{\mathbf{A}}(\mathbf{U}_0, \mathbf{U}_0) = \mathbf{A}(\mathbf{U}_0) = \left.\frac{\partial \mathbf{F}}{\partial \mathbf{U}}\right|_{\mathbf{U}=\mathbf{U}_0}$$

- **Conservation across discontinuities:**

$$\mathbf{F}(\mathbf{U}_\mathbf{R}) - \mathbf{F}(\mathbf{U}_\mathbf{L}) = \overline{\mathbf{A}}(\mathbf{U}_\mathbf{R} - \mathbf{U}_\mathbf{L})$$

Eigenstructure of MHD equation



- 7 wave speeds & 8 states.
- Slow / fast signals: might be shocks or rarefactions.
- Entropy wave: contact discontinuity.
- Eigenvalues $\lambda_k^{\pm}$ (wave speeds) may not be distinct.
- Right eigenvectors r_k (path taken in the phase space).
- Left eigenvectors l_k (charcteristic).

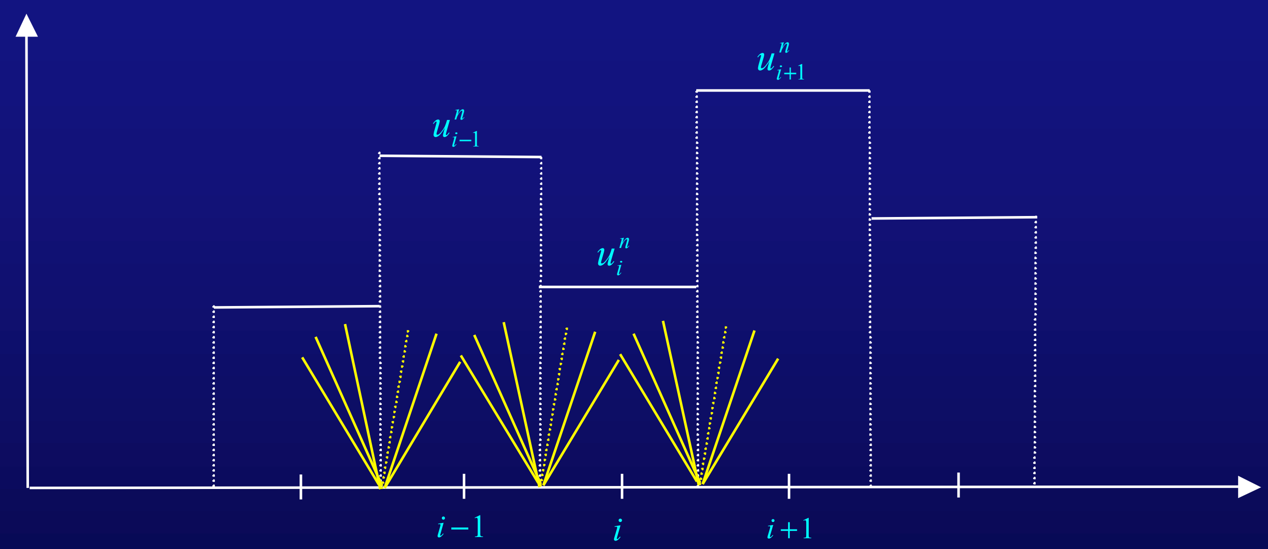
Intercell Fluxes of the Riemann Problem

Given $\quad \mathbf{U}(x,t^t) = \begin{cases} \mathbf{U}_L & \text{if } x < x_{i+1/2,j} \\ \mathbf{U}_R & \text{if } x > x_{i+1/2,j} \end{cases} \quad ,$

$$\mathbf{F}^*_{i+1/2,j}(\mathbf{U}_L,\mathbf{U}_R) = \frac{1}{2}\left[\mathbf{F}(\mathbf{U}_R) + \mathbf{F}(\mathbf{U}_L)\right] - \frac{1}{2}\sum_{k=1}^{7} |\lambda_k| \mathbf{l}_k \frac{\partial \mathbf{V}}{\partial \mathbf{U}} (\mathbf{U}_R - \mathbf{U}_L) \frac{\partial \mathbf{U}}{\partial \mathbf{V}} \mathbf{r}_k$$

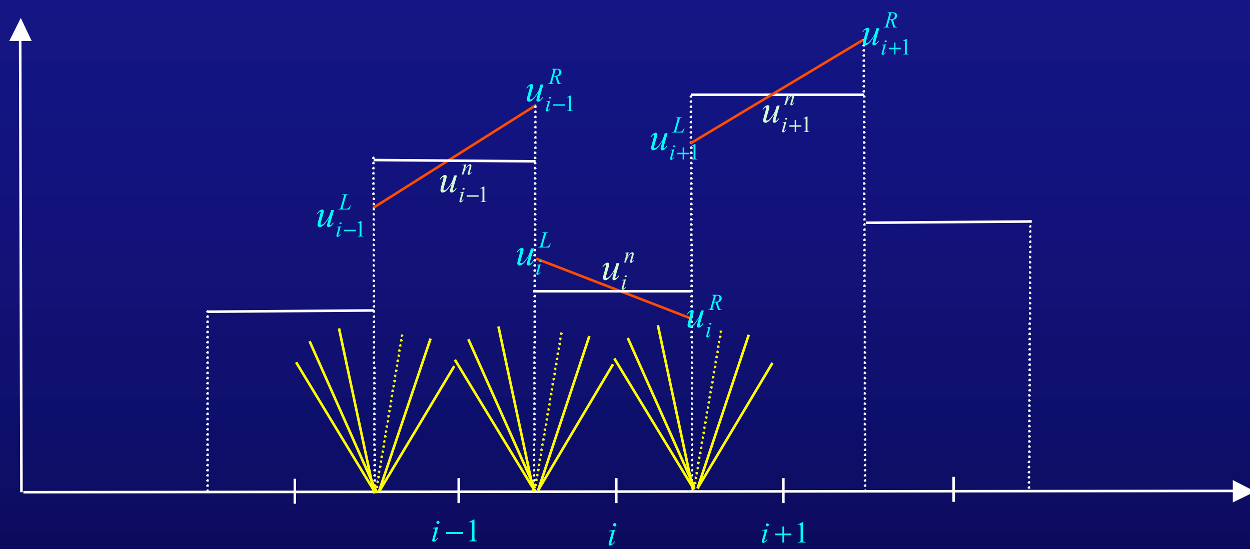
$$\mathbf{U}^{n+1}_{i,j} = \mathbf{U}^{n}_{i,j} - \frac{\Delta t}{\Delta x}\left[\mathbf{F}^*_{i+1/2,j} - \mathbf{F}^*_{i-1/2,j}\right] \qquad \text{in } x\text{-sweep}$$

First order Godunov method (FOG)



- Piecewise constantly distributed data at time level n.
- Solves Riemann problems at each intercell boundaries $i-\frac{1}{2}$ & $i+\frac{1}{2}$.

MUSCL-Hancock Method
- High order Godunov method (HOG)



- Data reconstruction: piecewise linearly distributed data at time level n,

$$u_i^L = u_i^n - \frac{1}{2}\overline{\Delta}_i \ \& \ u_i^R = u_i^n + \frac{1}{2}\overline{\Delta}_i$$

$$\overline{\Delta}_i = \begin{cases} \max[0, \min(\beta\Delta_{i-1/2}, \Delta_{i+1/2}), \min(\Delta_{i-1/2}, \beta\Delta_{i+1/2})], & \Delta_{i+1/2} > 0 \\ \min[0, \max(\beta\Delta_{i-1/2}, \Delta_{i+1/2}), \max(\Delta_{i-1/2}, \beta\Delta_{i+1/2})], & \Delta_{i+1/2} < 0 \end{cases}$$

- Time evolution:

$$\overline{u}_i^{L,R} = u_i^{L,R} - \frac{1}{2}\frac{\Delta t}{\Delta x}\left[F(u_i^R) - F(u_i^L)\right]$$

- Riemann problem with piecewise constant data: $(\overline{u}_i^R, \overline{u}_{i+1}^L)$

Dimensional splitting scheme in 2D

- First order accurate scheme: (Strang)

$$\left.\begin{array}{ll}\text{PDE}: & \mathbf{U}_t + \mathbf{F}(\mathbf{U})_x + \mathbf{G}(\mathbf{U})_y = 0 \\ \text{IC} \quad : & \mathbf{U}(x,y,t^n) = \mathbf{U}^n\end{array}\right\}$$

$$\Downarrow$$

$$\text{dimensional splitting}$$

$$\Downarrow$$

$$\left.\begin{array}{ll}\text{PDE}: & \mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = 0 \\ \text{IC} \quad : & \mathbf{U}^n\end{array}\right\} \overset{\Delta t}{\Longrightarrow} \mathbf{U}^{n+1/2} \quad (x\text{-sweep}, \mathrm{X}^{\Delta t}\text{-operator})$$

$$\left.\begin{array}{ll}\text{PDE}: & \mathbf{U}_t + \mathbf{G}(\mathbf{U})_x = 0 \\ \text{IC} \quad : & \mathbf{U}^{n+1/2}\end{array}\right\} \overset{\Delta t}{\Longrightarrow} \mathbf{U}^{n+1} \ (y\text{-sweep}, \mathrm{Y}^{\Delta t}\text{-operator})$$

Dimensional splitting scheme in 2D-cont'd

- Second order accurate scheme with 50% more work: (Strang)

$$\mathbf{U}^{n+1} = \mathbf{X}^{\Delta t/2}\mathbf{Y}^{\Delta t}\mathbf{X}^{\Delta t/2}\mathbf{U}^{n}$$

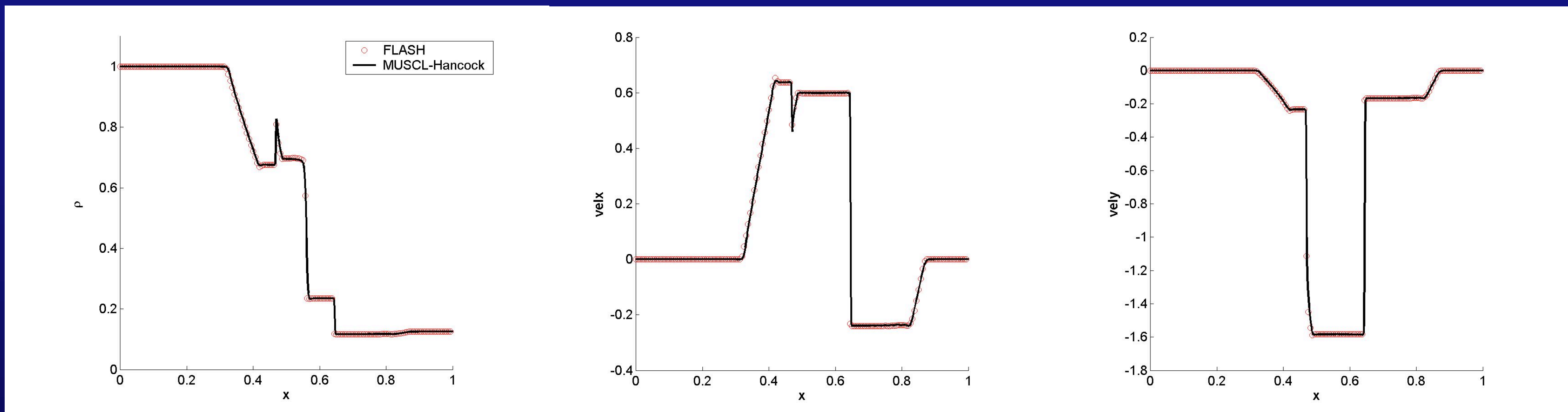
or

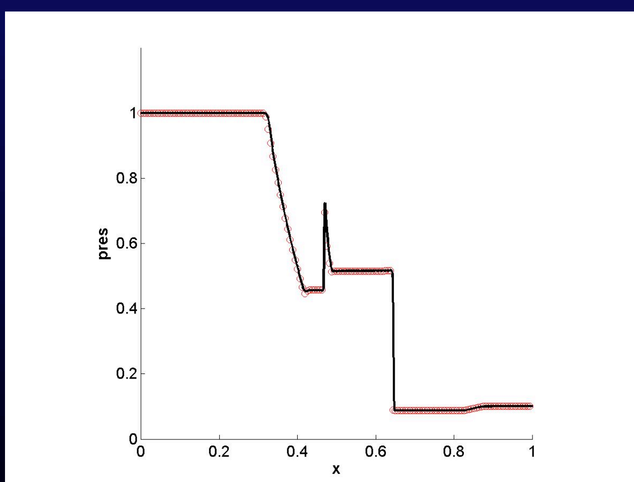
$$\mathbf{U}^{n+1} = \mathbf{Y}^{\Delta t/2}\mathbf{X}^{\Delta t}\mathbf{Y}^{\Delta t/2}\mathbf{U}^{n}$$

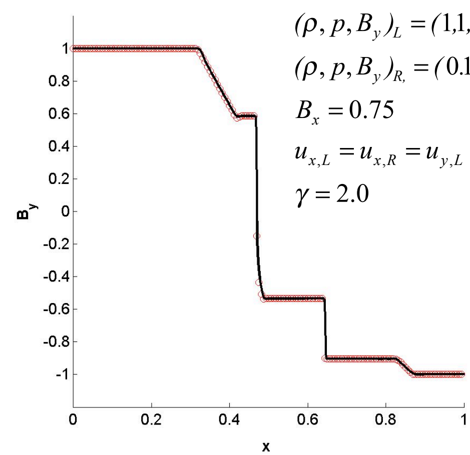
MHD Code at a glance

- Solves 1D and 2D MHD problems in the Cartesian grids.
- Written in Fortran 90 , started from scratch.
- 14 sub-modules with a driver (mhd.f90) routine, one runtime parameter file (mhd.init).
- One can choose from:
  - Outflow & periodic BC.
  - 1st and 2nd order (MUSCL-Hancock) Godunov methods.
  - w/ or w/o TVD, w/ or w/o entropy fix, two different averaging schemes.
  - Two different eigenstructures (Roe-Balsara & Ryu-Jones).
  - Control of a parameter β for different slope limiter functions (e.g., MINMOD, SUPERBEE).
  - 1st and 2nd order dimensional splitting schemes.
  - 3 different solution levels for 1D and 4 different levels for 2D.
  - Restart capability.
- Compile flags:
  - pgf90 –tpp7 –O2 in usual runs
  - pgf90 –g in debug mode

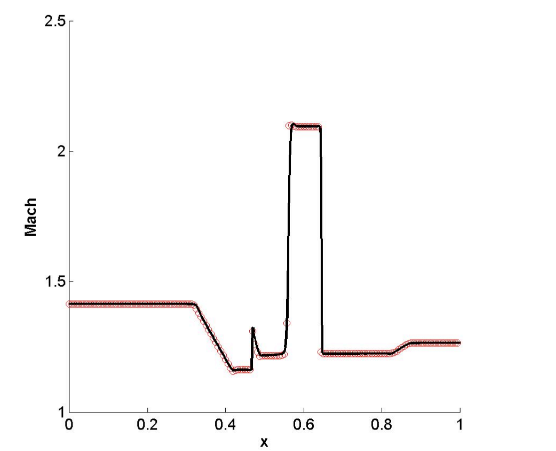
1D Brio-Wu problem - Verification study



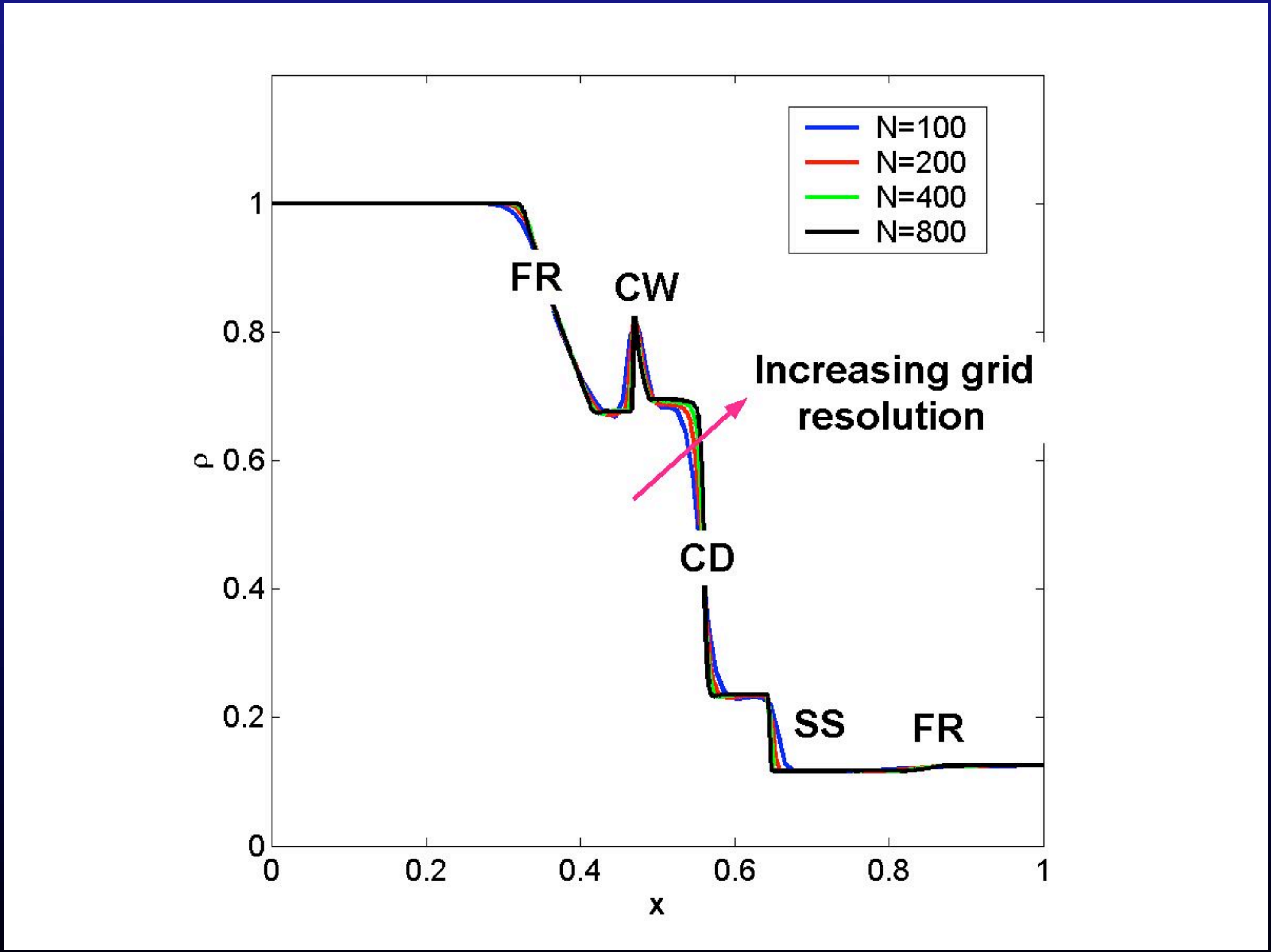




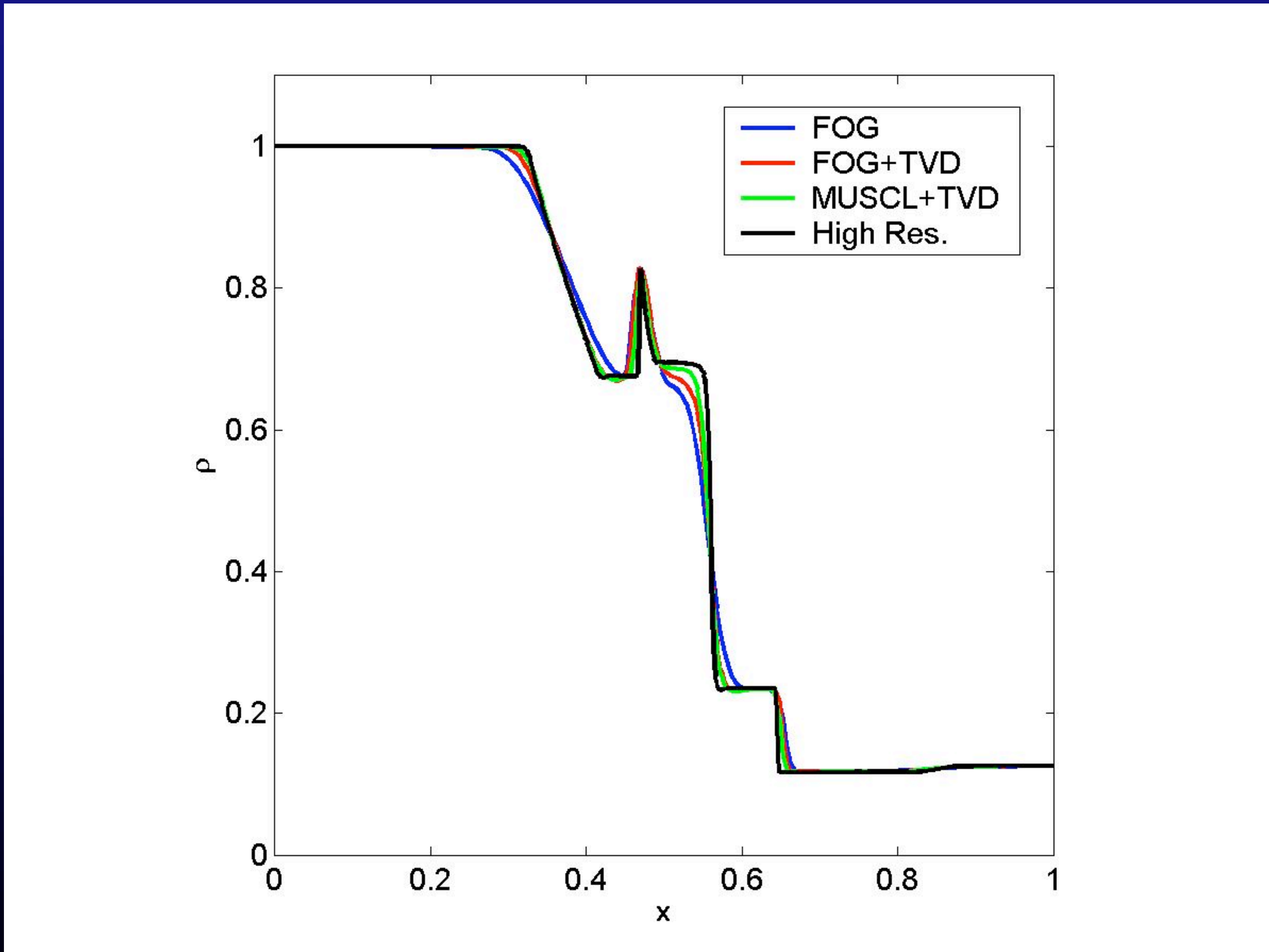
$$(\rho, p, B_y)_L = (1,1,1),$$
$$(\rho, p, B_y)_{R,} = (0.125, 0.1, -1),$$
$$B_x = 0.75$$
$$u_{x,L} = u_{x,R} = u_{y,L} = u_{y,R} = 0$$
$$\gamma = 2.0$$



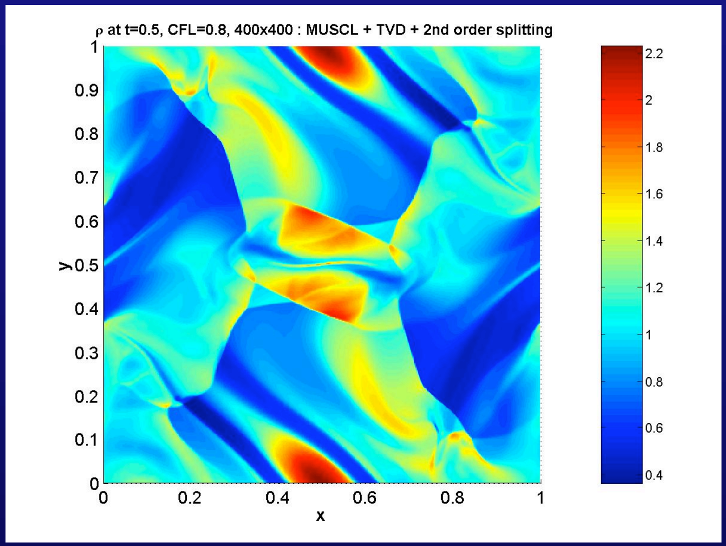
1D Brio-Wu problem – Grid resolution test

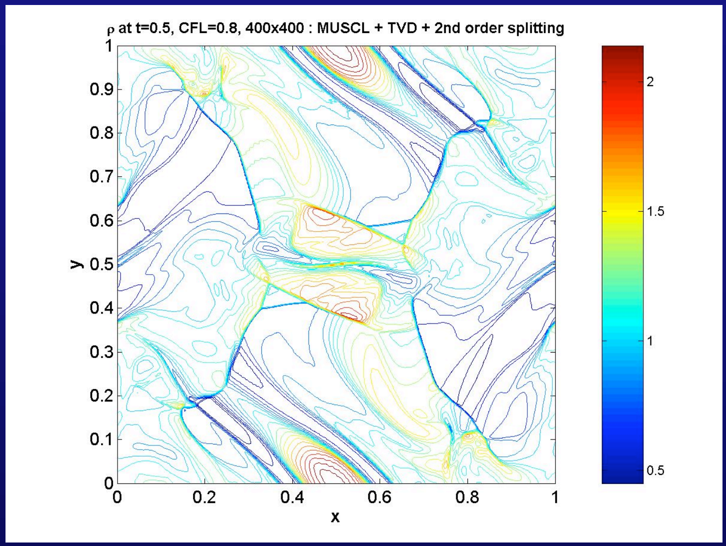


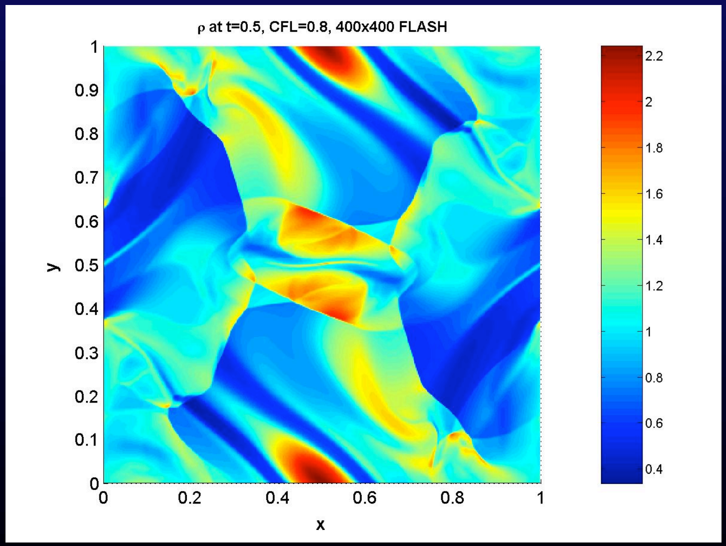
1D Brio-Wu problem – Sol'n level test (N=200)

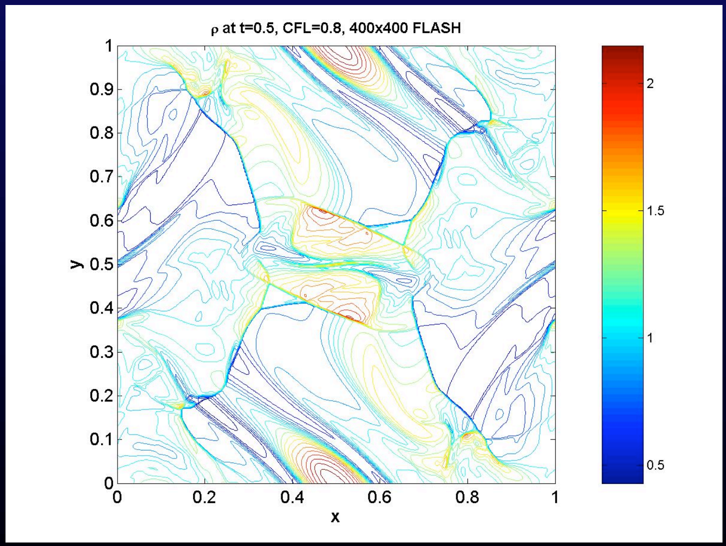


2D Orszag-Tang problem - Verification study

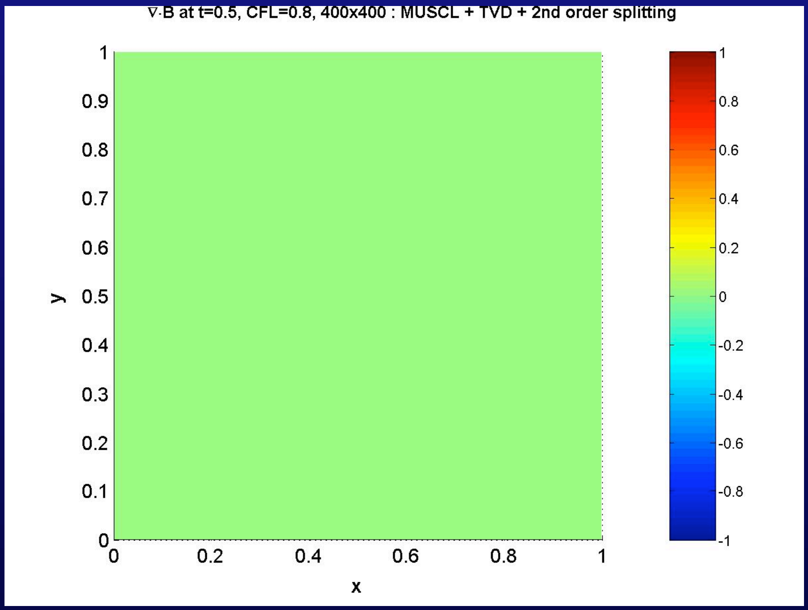


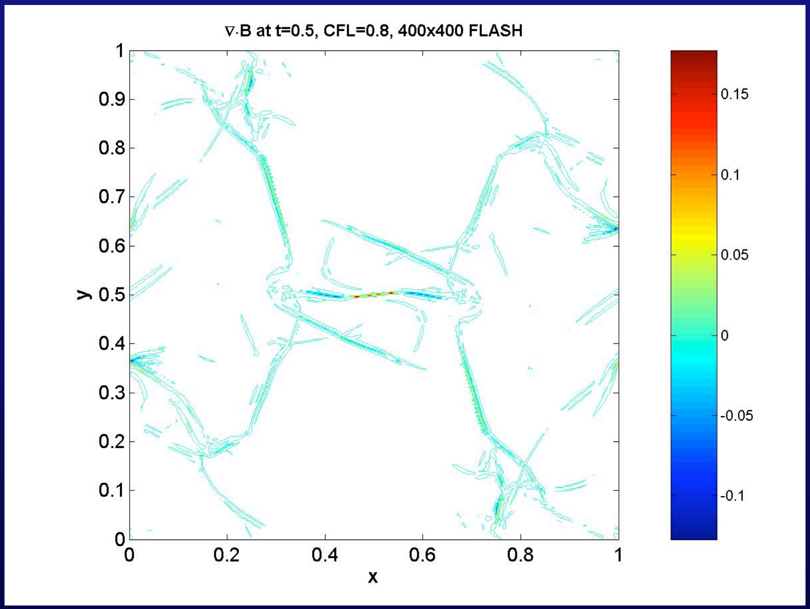






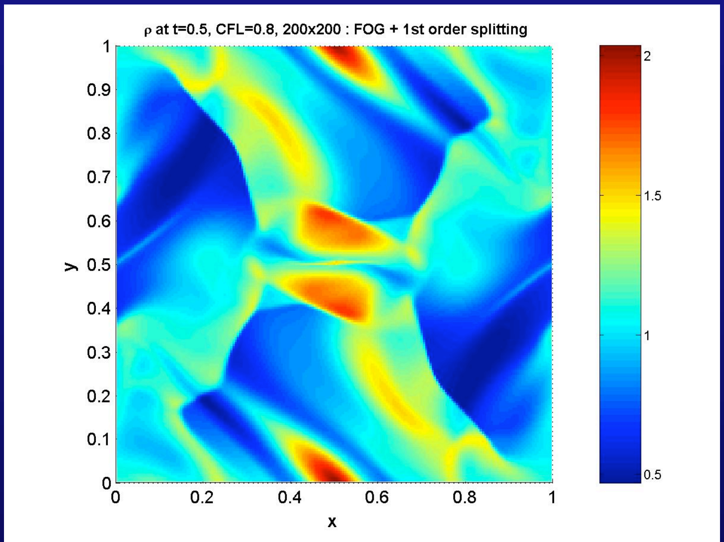
2D Orszag-Tang problem - Verification study

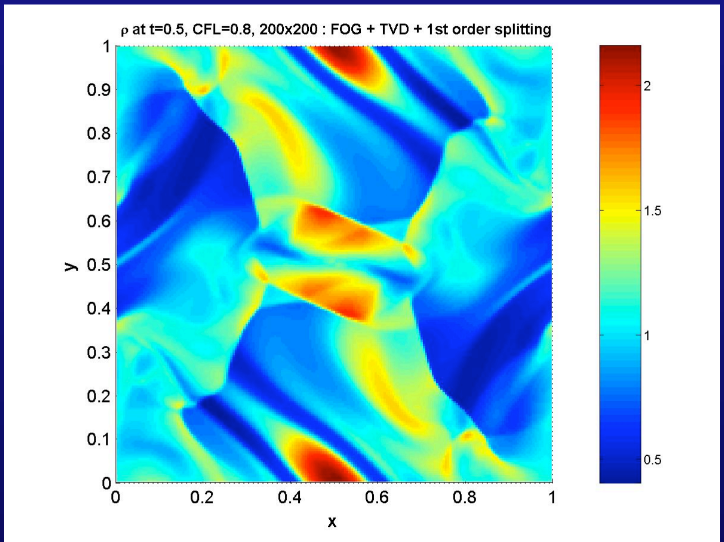


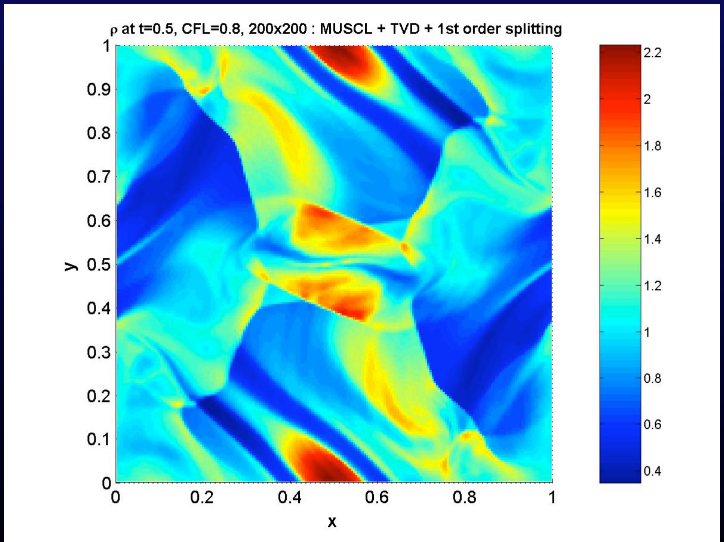


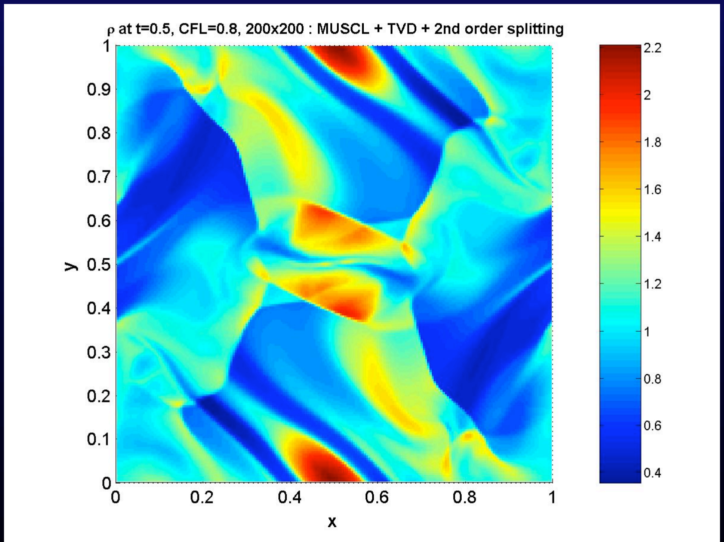
- Well validated results.
- Divergence free of magnetic fields are obtained using the staggered mesh algorithm, while nonzero values are evident in the FLASH results (8-wave scheme).

2D Orszag-Tang problem – Sol'n level test (200x200)





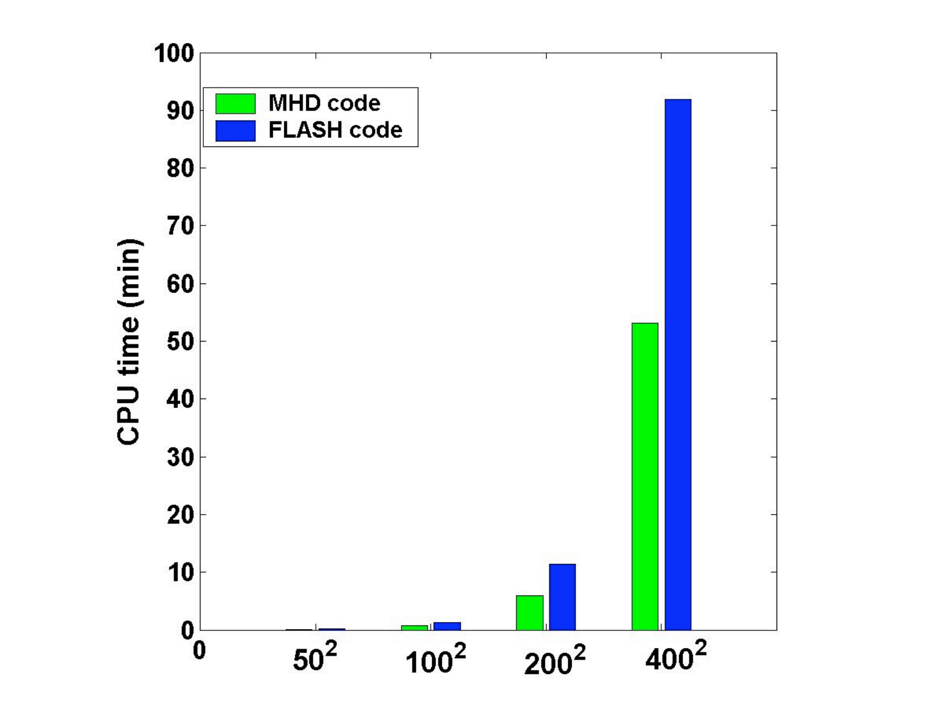




CPU Comparisons

- Average values of CPU time on a linux workstation of Pentium 4 2.4 GHz (2GB memory).

Grids	MHD code	FLASH code
50 x 50	6 sec	12 sec
100 x 100	49 sec	76 sec
200 x 200	356 sec	687 sec
400 x 400	5,512 sec	3,192 sec



2D Orszag-Tang problem – movie

- Density movie on 400x400 high resolution.
- CFL=0.8.
- 2nd order Godunov MUSCL-Hancock scheme.
- 2nd order accurate dimensional splitting in alternating order.
- Enjoy!

http://www.lcv.umd.edu/~dongwook/HTML/amsc663.htm

Conclusion & Future works

- Successful implementations of 1D and 2D MHD solver.
- Codes are well validated for well known bench marked problems, such as 1D Brio-Wu MHD shock tube problem and 2D Orszag-Tang MHD vortex problem.
- Compares well with the FLASH results.
- Performed systematic studies in data analysis.
- Keeps divergence of magnetic fields remain zero up to machine round-off errors throughout calculations, even for long period of time.
- Pure hydrodynamic problem can be considered as a limiting case.

- Implement other scheme (Crockett, Colella, et al., 2003) :
  - Unsplit scheme for accuracy
  - Projection method / Poisson solver
- 3D MHD turbulence problem:
  - Parallelization
  - AMR

References

1. Balsara, D. S., Spicer, D. S., ``A Staggered Mesh Algorithm Using High Order Godunov Fluxes to Ensure Solenoidal Magnetic Fields in Magnetohydrodynamic Simulation", *J. Comp. Phys.,* 149(1999), pp.~270-292.

2. Balsara, D. S., ``Divergence-Free Adaptive Mesh Refinement for Magnetohydrodynamics", *J. Comp. Phys*., 174(2001), pp.~614-648.

3. Toth, G., ``The $\nabla \bullet B = 0$ Constraint in Shock-Capturing Magnetohydrodynamics Codes", *J. Comp. Phys.,* 161(2000), pp.~605-656.

4. Toth, G., ``Computational Magnetohydrodynamics : Notes For An Introductory Level Course", http://hermes.elte.hu/~gtoth , June, 1998.

5. Brio, M., Wu, C. C., ``An Upwind Differencing Scheme for the Equations of Ideal Magnetohydrodynamics", *J. Comp. Phys., 75*(1988), pp.~400-422.

6. Orszag, A., Tang, C. M., ``Small-scale Structure of Two-Dimensional Magnetohydrodynamic Turbulence", *J. Fluid Mech*., 90, 129(1979).

7. FLASH, version 2.3, http://flash.uchicago.edu , June, 2003.

8. Stanchev, G., Zalesak, S., Deane, A., ``VizFlow", NASA Contractor Report CR-2003-212232 (2003), http://lcv.umd.edu/deane/

References – cont'd

9. Powell et al.,, ``A solution-Adaptive Upwind Scheme for Ideal Magnetohydrodynamics", *J. Comp. Phys.,* 154(1999), pp.~284-309.

10. Roe, P. L., Balsara, D. S., ``Notes on the Eigensystem of Magnetohydrodynamics",SIAM, *J. Appl. Math*., 56(1996), pp.~57-67.

11. Balsara, D. S., ``Linearized Formulation of the Riemann Problem for Adiabatic and Isothermal Magnetohydrodynamics $\nabla \bullet B = 0$", *The Astro. Physical Journal Supplement Series,* 116(1998), pp.~119-131.

12. Balsara, D. S., ``Total Variation Diminishing Scheme for Adiabatic and Isothermal Magnetohydrodynamics", *The Astro. Physical Journal Supplement Series,* 116(1998), pp.~133-153.